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Advanced CO_2 dispersion simulation technology for improved CCS safety

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Abstract

There is a risk of hazardous releases of CO_2 from Carbon Capture and Storage (CCS) facilities and infrastructure. To predict the exposure to the environment and to perform safety assessments, reliable and efficient simulation technology for detailed prediction of CO_2 dispersion in realistic, complex environments is needed. Here the development of an advanced industrial CO_2 dispersion simulation tool based on the CFD simulator KAMELEON FIREEX KFX® is discussed. The tool's capability of predicting CO_2 dispersion at realistic conditions has been demonstrated through relevant tests and comparisons of simulation results to experimental data from both laboratory tests and large-scale field trials.

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Keywords: carbon dioxide; dispersion modeling; complex geometries; CFD; KAMELEON FIREEX KFX

1. Introduction

Today a strong international research effort is put into the development of carbon dioxide (CO_2) capture, transportation and storage technologies as a strategy for reducing global CO_2 emissions from industry and power generation. When processing, transporting and storing large quantities of CO_2, there is a risk of hazardous releases of CO_2 into the atmosphere from blowdown vents and from accidental releases from process equipment, pipelines and

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storage tanks or caverns. At standard conditions, CO_2 is a colorless, odorless gas which is not detectable by human senses. However, the human body is very sensitive to changes in CO_2 concentrations, and the negative effects of CO_2 exposure on the human body depend both on the concentration levels and the exposure time. The US National Institute for Occupational Safety and Health (NIOSH) has set the Immediately Dangerous to Life and Health value (IDLH) for CO_2 to 4 % (molar basis) [1]. In addition to the hazard of asphyxiation due to released CO_2 displacing oxygen in the air, the inhalation of elevated concentrations of CO_2 can have toxic effects caused by increased acidity of the blood [2]. Furthermore, CO_2 is heavier than air and will replace air near the ground. Released CO_2 gas will typically follow the contours of the terrain and accumulate in valleys, pits and other topographic depressions and consequently represent a significant hazard to people and life in such areas. As CO_2, with regard to full-scale CCS, usually will be stored and transported at high pressures (in liquid or supercritical state), there are also other potential hazards related to accidental releases. A high-pressure release of CO_2 into the atmosphere will result in a high-momentum jet which by itself represents a hazardous situation. At the same time, strong Joule-Thomson cooling associated with high-pressure releases can give very low and potentially harmful temperatures in the near field.

Other substances, such as hydrocarbons, hydrogen sulfide (H_2S), carbon monoxide (CO) and various other impurities may also be present in CCS-related CO_2 streams. Some of these impurities may separately be far more dangerous to life and health than CO_2. For example, H_2S has an IDLH value of 0.01 % (molar basis). For gas mixtures at atmospheric conditions, the concentration levels of the various minor components are typically derived from the bulk gas flow in engineering gas dispersion calculations.

The planning, design and operation of CCS facilities and infrastructure require that the risk associated with handling large quantities of carbon dioxide is appropriately managed. Safety concerns will be a natural objection against CCS projects, and such projects need acceptance both by authorities and in the public opinion. It is therefore important to get a sound understanding of the consequences of operational releases and potential accidents as early as possible in the project planning.

In a hazard assessment, both the concentration levels and the time variation of the released CO_2 have to be known to quantify the CO_2 exposure. To predict the exposure to the environment, to perform safety assessments of CCS facilities and infrastructure and to pre-design safety measures, reliable and efficient simulation technology for detailed prediction of CO_2 dispersion in realistic, complex environments is needed.

Moreover, in industry application the problem owners and decision makers and the scientists often have very different background of practical and theoretical understanding. It is therefore vital that the simulation technology can be trusted and that it includes methods that can depict the results in such a way that decisions can be made by people with different knowledge or experience background.

Here, the development of a coherent simulation technology for safety assessment of both planned and accidental CO_2 releases from CCS-related activities will be demonstrated and discussed. The present development is based on the advanced fire and gas dispersion simulator KAMELEON FIREEX KFX® which is a result of about 40 years of research and development activities on turbulent flow and combustion at ComputIT, NTNU and SINTEF in Norway. KFX™ is basically a general purpose computational fluid dynamics (CFD) code with a wide operational domain, including three-dimensional transient simulation of flares, gas dispersion, fire development, fire mitigation and environmental flows under realistic conditions in complex geometries as well as in open terrain [3,4]. Coherent technology in this respect means similar operational platforms and no adjustable constants in the physical sub-models. A common understanding of the physical problem studied and the results is achieved in the simulator by extensive use of graphics and video animations. The KFX™ software is developed in cooperation with some of the world's largest oil and gas companies and is extensively validated. Today, KAMELEON FIREEX KFX® is recognized by major international oil and gas companies and by major operators in the risk management industry as a leading calculation tool for detailed fire simulations in realistic, complex geometries, and it is used in daily operation and production all over the world. In the present paper, the development of the KFX™ tool's ability to perform detailed three-dimensional transient numerical simulations of realistic CO_2 dispersion scenarios is discussed. An overview of CO_2 dispersion relevant KFX™ models and methods will be given. Validation is an essential part of the development of a practical simulation tool to document that the predictive tool is reliable and suited for its intended use. Examples from practical application of KFX™ and comparisons of KFX™ simulation results to data from both laboratory experiments and CO_2 dispersion field trials are presented.

2. Modeling CO_2 release and dispersion in KFX™

2.1. Release source modeling using comprehensive CO_2 thermodynamics

In hazard scenarios related to the CCS industry, complex phase transitions and flow patterns may occur during a release of CO_2 into the atmosphere. Carbon dioxide has a triple point at 5.18 bara and 216.59 K (-56.6°C), and its critical point is at 73.8 bara and 304.13 K (31.0°C). At normal atmospheric pressure, pure CO_2 may exist in the gas phase, in the solid phase or as a mixture of gas and solids. At the standard state, carbon dioxide is stable in the gas phase, and solid CO_2 existing at these conditions will eventually sublimate. For technical and economic reasons, CO_2 is usually compressed into liquid or supercritical state before transport and storage. An accidental high-pressure CO_2 release may therefore typically result in a very complex high-momentum multiphase flow which includes formation of solid CO_2 particles which disperse, sublimate and possibly deposit downstream the release point. This may have a significant influence on the CO_2 doses (representing the combined effect of concentration and exposure time) in the near field and in the far field of an accidental release, in addition to possible near field cooling hazards. A proper model for high-pressure CO_2 releases that accounts for subsequent mass and heat transfer during phase transitions is therefore needed to obtain reliable and accurate dispersion predictions.

For consequence analyses of high-pressure releases of CO_2, one is often much more interested in the overall dispersion of the resulting CO_2 cloud than in the details of the complex flow structure of the underexpanded jet at the release point. For CFD dispersion simulations of practical interest, both adequate accuracy and considerably reduced computational costs can be achieved through the use of a so-called pseudo-source model (a release source model). In the pseudo-source concept, the expansion process is modeled at subgrid level to calculate equivalent expanded flow characteristics at atmospheric conditions. Here a pseudo-source model for CO_2 has been developed to calculate equivalent expanded flow parameters to be used as inlet conditions for the subsequent CO_2 dispersion simulation with KAMELEON FIREEX KFX®. The pseudo-source model employs fundamental physical principles of conservation of mass, momentum and energy for a control volume, and homogeneous equilibrium conditions are assumed during the expansion process. For the high-pressure CO_2 release modeling in the present work, an isentropic expansion process is assumed from stagnation conditions to the flow conditions at the outlet orifice, and an isenthalpic expansion process is assumed from the orifice to the equivalent exit conditions at atmospheric pressure. To calculate the equivalent exit parameters, a thermodynamic basis for handling the CO_2 expansion process from high-pressure conditions to atmospheric conditions involving real fluid and solid-state CO_2 thermodynamics has to be established.

For the CO_2 release-source modeling in KFX™, comprehensive and accurate equations of state and relevant auxiliary equations for carbon dioxide in the gas, liquid and solid phase have been included. For calculation of fluid properties of CO_2, Span and Wagner's equation of state is used together with auxiliary thermodynamic property equations for the saturation pressure, saturated liquid density and saturated vapor density [5]. Span and Wagner's equation of state for CO_2 is internationally recognized as a reference equation representing even the most accurate experimental data within their experimental uncertainty. It is valid from the triple-point temperature to 1100 K at pressures up to 800 MPa. It is formulated as a fundamental thermodynamic function for CO_2 explicit in the dimensionless Helmholtz energy and split into an ideal-gas part and a part accounting for residual fluid behavior. Span and Wagner determined the residual fluid part through sophisticated multi-property fitting procedures and optimization of the structure of empirical correlation equations based on more than 5000 experimental data points.

For the calculation of solid state properties of CO_2, the equation of state developed by Jäger and Span [6] has been applied. This equation is reported to be valid in the region from 0 MPa to 500 MPa and from 80 K to 300 K. It is formulated as a fundamental thermodynamic function for CO_2 explicit in the Gibbs free energy, and it is able to represent most of the available thermodynamic data for the CO_2 solid state within the uncertainty of the experimental data.

In addition, some auxiliary thermodynamic equations are used in the CO_2 release-source modeling in KFX™; an equation for the sublimation pressure and its derivative with respect to temperature reported by Trusler [7] and Plank and Kuprianoff's equation for the vapor enthalpy of CO_2 valid from 0 to 35 ata [8], which was modified to match the specific enthalpy at the triple point given by Span and Wagner [5].

2.2. Multiphase CO_2 dispersion modeling

An Euler-Lagrange model has been developed and used to simulate multiphase CO_2 dispersion with KAMELEON FIREEX KFX®. For high-pressure releases of CO_2, necessary flow input parameters for the release source in the Euler-Lagrange dispersion model are calculated by the pseudo-source model for an equivalent release at atmospheric conditions.

In KFX™ dispersion simulations, the gas phase typically consists of various gas components using an ideal-gas approximation. The gas phase flow behavior is modeled by the Reynolds-averaged partial differential equations for conservation of mass (species), momentum and energy for time-dependent three-dimensional turbulent flow in a gravitational field. Turbulence is modeled by the k-epsilon model with standard constants [9] and extended for effects of turbulence production due to buoyancy. Wall laws for the turbulent boundary layer are applied to calculate wall shear stress and convective heat transfer coefficients. The wall-law models are represented as source terms in the momentum equations, turbulence equations and energy equation.

Dispersion and sublimation of solid CO_2 particles is modeled by a Lagrangian particle spray model which is fully coupled to the Eulerian treatment of the gas phase flow. In the KFX™ Lagrangian spray model, numerical "parcels" of liquid droplets and/or solid particles are followed. One such numerical parcel of droplets/particles represents a class of physical droplets/particles with similar physical characteristics, i.e. each numerical parcel consists of droplets/particles with identical position, velocity, size and temperature. For each parcel of droplets/particles, eight differential equations are solved; three equations for the position (trajectory), three equations for the velocity (momentum), one equation for the droplet/particle mass and one equation for the droplet/particle temperature (energy). In the KFX™ spray model framework, droplet and/or particle distributions can be handled. The spray model includes an evaporation model and a sublimation model for droplets and particles, respectively. Furthermore, droplets and/or particles hitting an object may cool (or heat) the object and drip/fall, and a liquid water pool or a dry ice bank may be formed on surfaces. Hence, the present Euler-Lagrange model handles the dispersion of CO_2 particles, including flow interactions between the gas and solid phase, and accounts for mass and heat transfer during sublimation of solid particles of CO_2. Entrainment of ambient air into the CO_2 stream is inherently handled by the model. Effects of water-based mitigation systems, e.g. water curtains, can also be modeled using the spray model in KFX™.

2.3. Wind modeling

Appropriate wind boundary conditions are in general important in dispersion simulations of practical interest. Realistic atmospheric wind profiles and turbulence information may sometimes be approximated from wind measurement data, but in most engineering CFD studies, wind inlet profiles and wind turbulence data are assumed from empirically based theoretical analyses of the atmospheric boundary layer, such as the Monin-Obukhov similarity theory for the atmospheric surface layer, see e.g. work by Van Ulden and Holtslag [10] and Duynkerke [11]. Such logarithmic wind profiles are also applied in KAMELEON FIREEX KFX®, where profiles for wind velocity, turbulence energy and rate of dissipation of turbulence energy are specified on the boundary of the computational domain based on a prescribed wind velocity at a given reference height, a Monin-Obukhov length scale, a roughness scaling height, the current latitude for calculation of Coriolis effects and the wind temperature. Further, the Monin-Obukhov length scale can be estimated based on the Pasquill class for atmospheric stability, where the present implementation in KFX™ is valid for neutral and stable wind conditions.

For a high-pressure release of CO_2 resulting in a high-momentum jet, the effects of wind conditions will be limited in the near field close to the release point. For low-momentum releases or when the momentum-driven flow associated with the release source is weakened, the nature of a dense gas release of CO_2 typically turns into a gravity-driven flow where a gas cloud forms and expands, closely following the terrain, with a characteristic elevated gas cloud edge. At this point, atmospheric turbulence has limited influence on the dense gas cloud. The turbulence within the gas cloud will typically be different from the turbulence in the surrounding atmosphere, and the gas in the characteristic vortex ring at the edge of the cloud will appear more or less undiluted. However, some mixing will occur at the interface between the surrounding air and the dense CO_2 gas. Eventually, this vortex ring

collapses and the atmospheric turbulence becomes more and more important for the downstream dispersion of the released gas.

2.4. Complex geometries and terrain modeling

Appropriate modeling of terrain and complex geometries is essential if reliable CO_2 dispersion predictions for realistic industrial scenarios are expected. In KFX™ solid elements are rigorously treated and the consequences for mass, momentum and energy of the fluid are accounted for according to the physical processes involved. Objects less than the grid spacing are approximated by volume and/or surface porosities which generate for instance restrictions to the flow field and thermal radiation through such volumes, and are included when solving the governing equations. Thermal effects of the porosities are also accounted for. In KFX™ the geometry modeling is based on import of CAD models, and the porosities are automatically calculated on this basis.

Often, body-fitted computational grids are recommended for CFD simulations of complex shapes. However, there are practical limits regarding the complexity of the shapes that can be handled effectively with body-fitted grids. To create a body-fitted grid for a process plant is in itself a complicated calculation that would be too time-consuming to be practicable. Today, most industrial CFD studies involving complex geometries in large physical domains apply Cartesian computational grids. Fluid flow simulations within, on and around complex geometries will then often involve fluid flow along surfaces which are not aligned with the grid lines of the calculation domain. When a Cartesian computational grid is applied, skew surfaces are approximated by blocked-off rectangular volumes in a staircase pattern. By default, this approach leads to strong non-physical friction or false diffusion along the skew surfaces and will represent a source of error in dispersion simulations. A method that compensates for this false diffusion adjacent to skew solid surfaces is implemented in KFX™, where this kind of false diffusion is avoided by modifying the numerical approximation adjacent to the skew surface.

3. Computational elements of KFX™

In addition to being able to give reliable predictions, advanced industrial simulation tools need also to be efficient, numerically stable and robust. Today, a quantitative risk analysis of a gas industry plant may involve from several hundred to possibly several thousand dispersion simulations, and computational costs must therefore be controlled and balanced against the need for sufficiently accurate predictions for practical applications.

- KAMELEON FIREEX KFX® is an industrial finite-volume CFD code which solves the fundamental conservation equations for three-dimensional time-dependent turbulent flow and combustion using a non-uniform Cartesian grid.
- The grid system can be generated automatically or manually.
- A large number of special cells have been developed for boundary conditions of practical interest. For instance, KFX™ includes pool spreading models and special cells for high-pressure gas releases.
- KFX™ includes powerful CAD import capabilities where CAD geometries, including electronic maps of terrain, buildings, modules, process plants, pipelines, etc. are converted automatically into computational cells for solid constructions or surface/volume porosities used by the KFX™ calculation model.
- A multi-block solution technique has also been developed and implemented to enable flexibility and refined predictions in different regions of the computational domain without increasing the computational costs beyond acceptable limits. For industrial CO_2 dispersion hazard scenarios, this means an improved ability to predict both the near field and the far field of the computational domain more accurately.
- KFX™ includes a user interface which is designed to reduce simulation set-up times and possibilities of operator errors.
- Results can be presented in a number of different ways, including visualizations in the CAD geometry.
- Videos can be generated at observation points inside and outside the computational domain.
- KFX™ is interfaced with structure response models.

4. Examples from model testing and validation

To verify and document that the predictive simulation tool is reliable and suited for its intended use, comparisons of simulation results to experimental data are vital. Validation is a continuously ongoing and very important activity in the development of the KAMELEON FIREEX KFX® simulation tool. The CO_2 specific model developments are based on a tested and validated framework of general numerical methods and physical models for CFD simulations of fire and gas dispersion. In general, KFX™ has been extensively validated at several different levels [4]:

- against analytical solutions
- against scientific experiments with a high degree of accuracy
- against realistic full-scale tests
- through sub-model tests
- through integrated tests
- through small-scale, medium-scale and large-scale tests
- through blind tests and "full-information" tests

For CCS relevant CO_2 dispersion modeling, including the possibility of multiphase CO_2 flow into the surroundings, specific tests and validation work have been performed [12]. Both sub-model and integrated tests have been performed. KFX™ predictions have been compared to results from both wind tunnel CO_2 dispersion experiments and large-scale CO_2 field experiments. In the following, some examples from this validation work are given, and some illustrative simulation results from a large-scale accident scenario are presented.

4.1. Tests of the thermodynamic property model implemented in the KFX™ pseudo-source model

Numerical predictions of CO_2 mass density, specific enthalpy and specific entropy by the comprehensive CO_2 thermodynamic property model implemented in the KFX™ pseudo-source model were compared to data for various thermodynamic states given in the work by Span and Wagner [5]. Excellent agreement between the KFX™ model predictions and the thermodynamic data were observed [12]. Excellent agreement between the predicted heat of sublimation at the sublimation point (194.67 K) and the corresponding measured value by Giauque and Egan [13] was also observed [12].

A comparison of predicted and measured initial mass density of CO_2 contained in a 6.3 m^3 test vessel used in large-scale Shell CO_2 experiments in 2010 [14] is presented in Table 1 below.

Table 1. Measured and predicted initial density of CO_2 in Shell test vessel

Shell Test No.	1	2	4	14	16
Storage state	liquid	liquid	liquid	supercritical	supercritical
Pressure (bar)	149.3	148.1	149.2	152.6	151.6
Temperature (K)	299.85	297.75	293.25	344.15	309.85
Measured density (kg/m^3)	890	919	907	493	826
Predicted density (kg/m^3)	866	877	903	509	806
Deviation (%)	-2.7	-4.6	-0.5	3.1	-2.5

The results show very good agreement between the KFX™ predictions and the measurements of the initial CO_2 densities in the test vessel.

A comparison of predicted and measured initial CO_2 mass flow rates was also performed for 9 large-scale CO_2 experiments where the releases were modeled as so-called true orifice releases based on the pressure and temperature at the test vessel outlet (i.e. ignoring friction upstream of the orifice) [12]. Close agreement between predicted and measured mass flow rates was found for the majority of the tests. However, a deviation in the range from 15.7 % to 21.3 % (absolute values) was observed for some of the tests. The observed deviations may be

attributed to several factors. For example, the thermodynamic expansion process assumptions represent a simplification of the complex reality. The discharge modeling was performed with a chosen orifice discharge coefficient of 0.6 in these tests. For the test where the largest deviation was observed, it was noted that a discharge coefficient of 0.76 instead of 0.6 would give a predicted mass flow rate equal to the reported mass flow rate from the measurements. In some tests the specified initial pressure used in the prediction may also have been too high as frictional effects upstream of the orifice may be significant. Though simplified modeling of the flow expansion process may be a plausible cause of deviations between predictions and experiments, both lack of necessary model input data and experimental errors should also be considered. For instance, in the large-scale BP CO_2 experiments [15] the reported CO_2 mass flow rates were estimated based on measured vessel weight using load cells. A significant inaccuracy is therefore likely to be found in these estimates, cf. the critical reviews by Witlox [14, 15]. Mass flow rates from Coriolis flow meter measurements, as in the large-scale Shell CO_2 experiments [14], are considered to be more accurate. Overall, the agreement between the predicted and the measured mass flow rates was considered to be relatively good, considering both the uncertainties of the derived mass flow rates and the model assumptions.

The amount of solid CO_2 formed in an atmospheric release will affect the nature of the subsequent dispersion process. Mass fractions of solid CO_2 formed at atmospheric pressure from 12 large-scale high-pressure CO_2 releases have therefore been predicted by KFX^{TM} and compared to predictions by DNV [14, 15]. Generally, an excellent agreement between the two different models for the predicted solid CO_2 mass fractions was observed [12].

4.2. Three-dimensional simulations of wind tunnel CO_2 dispersion tests

A series of wind tunnel experiments on dispersion of CO_2 gas has been simulated with KFX^{TM}. In the experiments, conducted by the Chemical Hazards Research Center (CHRC) at the University of Arkansas (USA) in 2006, wind tunnel data from three experimental configurations were produced [16]:

- Test A: A low-momentum area source CO_2 release (vertical) without obstacles
- Test B: A low-momentum area source CO_2 release (vertical) with a tank and a dike
- Test C: A low-momentum area source CO_2 release (vertical) with a dike only

The CHRC facility is an ultra-low-speed boundary layer wind tunnel capable of producing airflows that simulate the constant stress layer of the atmospheric boundary layer. The test section dimensions were 2.1 m by 6.1 m by 24.4 m. The wind tunnel floor consisted of rubber matting with mounted roughness elements, to give turbulence properties consistent with field-scale scenarios. Room-temperature CO_2 was released continuously, at a rate of 33.4 standard liters per minute (slpm) with 0.5 slpm C_3H_8 added as a tracer, through a square-shaped area with a central circular section blocked off. The measured wind speed was 0.4 m/s at a reference height of 6.7 cm. Gas concentration measurements were made at an elevation of 0.5 cm, at several downwind distances from the source and with 10 cm spacing in the transversal direction. In the obstructed tests, a square-shaped dike with an inner dimension of 63 cm and a wall height of 3.7 cm was used. The tank in Test B consisted of a 31 cm-diameter vertical cylinder with a spherical dome top with a total height of 28.3 cm. The tank was located in the center of the dike. The gas was released through a meshed screen from the area inside the dike. The KFX^{TM} geometry model of the experimental setup for Test B is shown in Fig. 1. More details on the CHRC CO_2 dispersion experiments are given by Havens and Spicer [16].

In the simulations, KFX^{TM} wind inlet profiles corresponding to neutral atmospheric stability conditions (stability class D) were applied. Furthermore, to reduce the simulation times, the nominal symmetrical geometry of the test setups was exploited by simulating half of the physical domain through application of a symmetrical boundary in the computational domain. A relatively fine computational grid was used in the simulations to capture the influence of the small geometrical objects on the measurement points in these wind-tunnel dispersion tests. The computational domain consisted of approximately $3.4 \cdot 10^6$ computational cells.

The detailed KFX^{TM} predictions and the corresponding measurements showed overall good agreement for the three wind tunnel CO_2 dispersion tests [12]. Figure 2 shows the predicted horizontal iso-contours of CO_2 mole

fractions (%) at 5 mm above the wind tunnel floor for Test B. The predicted vertical iso-contours of CO_2 mole fractions (%) in the center of the wind tunnel for the same test are shown in Fig. 3.

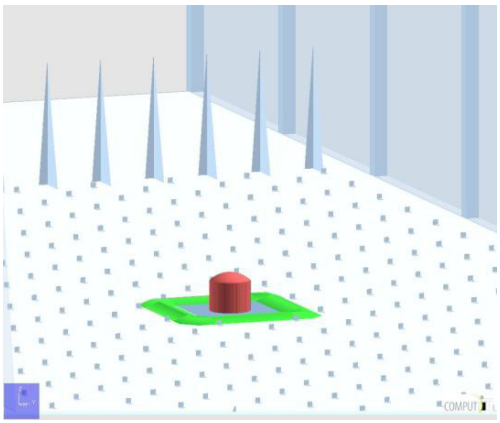

Fig. 1. KFX^{TM} geometry model of CHRC Test B, showing CO_2 inlet configuration.

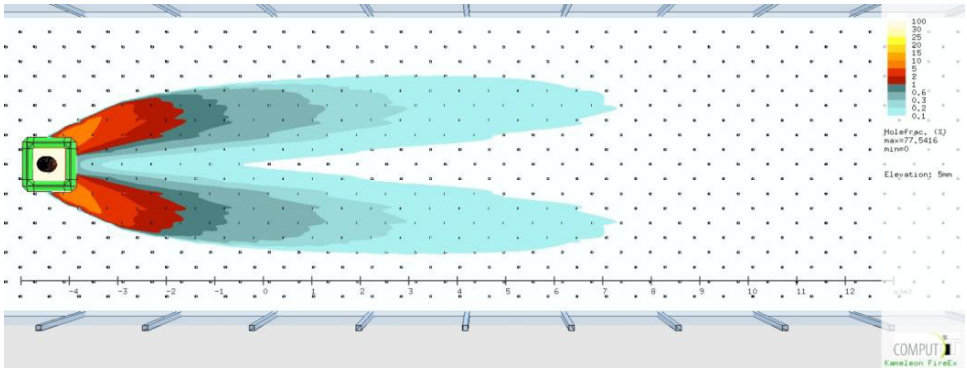

Fig. 2. Predicted horizontal iso-contours of CO_2 mole fractions (%), 5 mm above the wind tunnel floor, CHRC Test B.

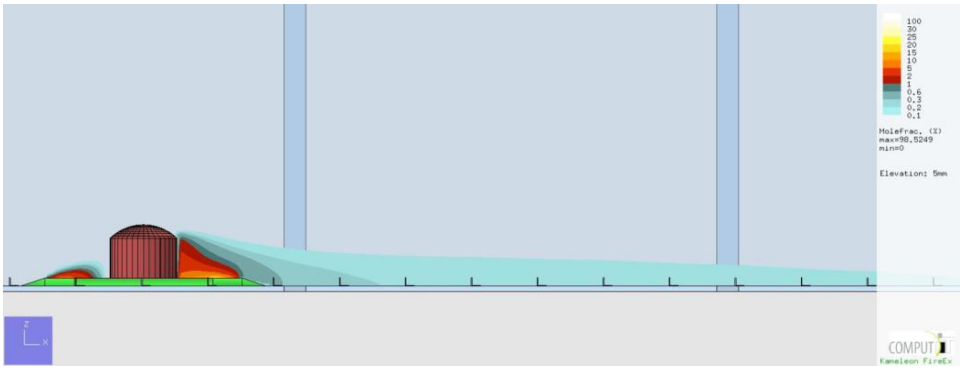

Fig. 3. Predicted vertical iso-contours of CO_2 mole fractions (%), in the center of the wind tunnel, CHRC Test B.

As seen in Fig. 2 and Fig. 3, the geometry affects the CO_2 dispersion significantly. The predicted bifurcation of the gas cloud for Test B is in good agreement with the reported experimental observations [16]. More information on the detailed comparison of the KFX™ simulation results to the experimental data from the wind tunnel tests is given in [12].

4.3. Three-dimensional simulations of the BP and Shell large-scale CO_2 dispersion tests

A substantial amount of experimental data from large-scale CO_2 field experiments was released by the DNV led CO2PIPETRANS joint industry project in 2012 to support CO_2 dispersion model validation [17, 18]. A description of a selection of horizontal free releases of liquid CO_2 and a comparison of KFX™ simulation results to experimental data is given here.

A series of field experiments to study the flow and dispersion of high-pressure releases of dense phase carbon dioxide was conducted by Advantica under contract to BP Alternative Energy Ltd at the Spadeadam test site in the UK in 2006. In these BP tests [17, 19, 15], the dense phase CO_2 was released horizontally, 1.1 m above a designated nominally flat concrete pad (Pad A) where an array of downstream field detectors for measurement of concentrations and temperatures were located. The reported carbon dioxide concentrations were primarily derived from measured reduction in oxygen concentration monitored by oxygen cells at up to 43 locations, with sensor locations at downstream distances of 5-80 m and cross-stream distances between -20 and +20 degrees. Most of the sensors were positioned 1 m above the concrete pad with some additional measurements at heights of 0.3 m and 3.0 m. Detailed information on the BP test setup and the measurements can be found in the reports by Holt [17], Evans and Graham [19] and Witlox [15]. A KFX™ geometry model for the horizontal free release tests is shown in Fig. 4.

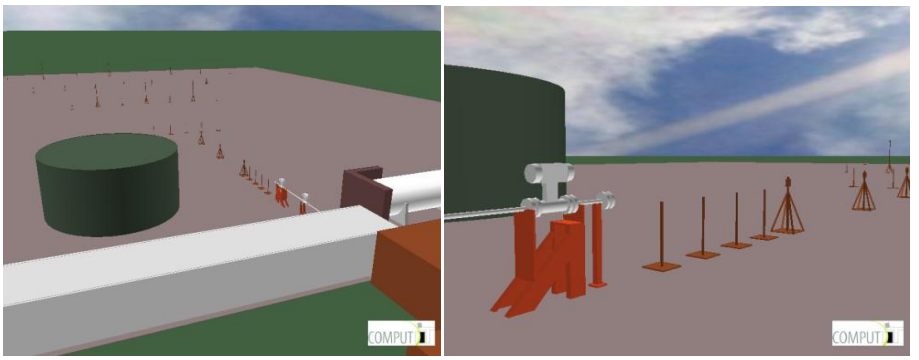

Fig. 4. Snapshots of the KFX™ geometry model for the BP CO_2 release tests.

In 2010, a new series of large-scale CO_2 release and dispersion tests sponsored by Shell was executed using the same rig at the Spadeadam test site, which now was operated by GL Noble Denton. Based on the experience from the previous BP tests, some modifications were done in the Shell tests. Additional concentration and temperature measurements were performed as well. In these tests, the center of the discharge orifice for the horizontal free releases was located 1.0 m above the concrete pad. Detailed information on the Shell test setup and the measurements can be found in the reports by Holt [18], Allason and Armstrong [20] and Witlox [14].

KFX™ validation simulations have been performed for BP CO_2 dispersion Test No. 1, 2, 5 and 11, see Table 2. Further, KFX™ validation simulations have also been performed for Shell CO_2 dispersion Test No. 3, 5 and 11, see Table 3. For all simulation cases, CO_2 stored in a liquid state was released into the atmosphere, which resulted in multiphase dispersion of CO_2 gas and solid particles. In these tests, the average ambient temperature ranged from 277 K to 287 K and the average wind speed ranged from 1.3 m/s to 6.4 m/s (at 10 m above the ground). The wind was blowing in various directions for each of these tests, i.e. in the direction of the release ± 57°. In the simulations, KFX™ wind inlet profiles corresponding to neutral atmospheric stability conditions (stability class D) were applied.

The computational domain consisted of approximately $1.88 \cdot 10^6$ computational cells. In addition, for the two-phase release-source modeling of the equivalent atmospheric release conditions, up to 100 000 numerical parcels of monodisperse solid CO_2 particles were released per second into the computational domain during the transient three-dimensional simulations. Further information on the simulation setup and detailed validation results are given in [12].

Table 2. BP CO_2 dispersion tests simulated with KFX™

BP Test No.	1	2	5	11
Initial storage pressure (bar)	103.4	155.4	156.9	82.2
Initial storage temperature (K)	278.35	281.85	285.65	291.55
Release orifice diameter (mm)	12.7	12.7	25.4	12.7
Mass flow rate, measured (kg/s)	8.2	11.4	40.7	7.1

Table 3. Shell CO_2 dispersion tests simulated with KFX™

Shell Test No.	3	5	11
Initial storage pressure (bar)	153.0	131.6	82.9
Initial storage temperature (K)	282.1	286.95	272.95
Release orifice diameter (mm)	12.7	25.4	12.7
Mass flow rate, measured (kg/s)	12.6	45.6	8.9

The predicted multiphase dispersion of CO_2 from the dense phase release in BP Test No. 2 is illustrated in Fig.5. Note that the size of the CO_2 particles is not to scale in this plot, but light particle colors represent smaller particles. As expected, it can be observed that the resulting cold, dense gas cloud drops to the ground as the initial momentum of the jet decreases. It is also seen that KFX™ predicts that the CO_2 particles sublimate before they reach the ground. This is in accordance with the observations made at the test site.

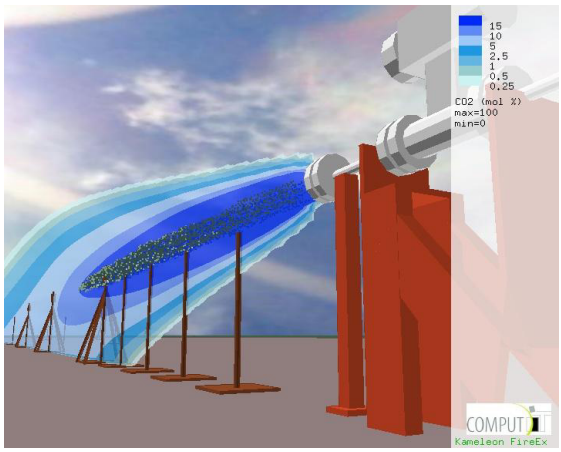

Fig. 5. Predicted gas concentrations of CO_2 (mol %) in a vertical cross-section through the dense phase CO_2 release, including visualization of the small dry ice particles in the gas flow. BP Test No. 2.

In Fig. 6, the maximum predicted mole fractions of CO_2 at different downstream distances from the release point are compared to the corresponding measured maximum mole fractions of CO_2 (11-second averaged) for the BP CO_2 dispersion tests. A corresponding comparison for the Shell CO_2 dispersion tests is shown in Fig.7. For consistency, all predicted maximum mole fractions of CO_2 are taken at the measurement points.

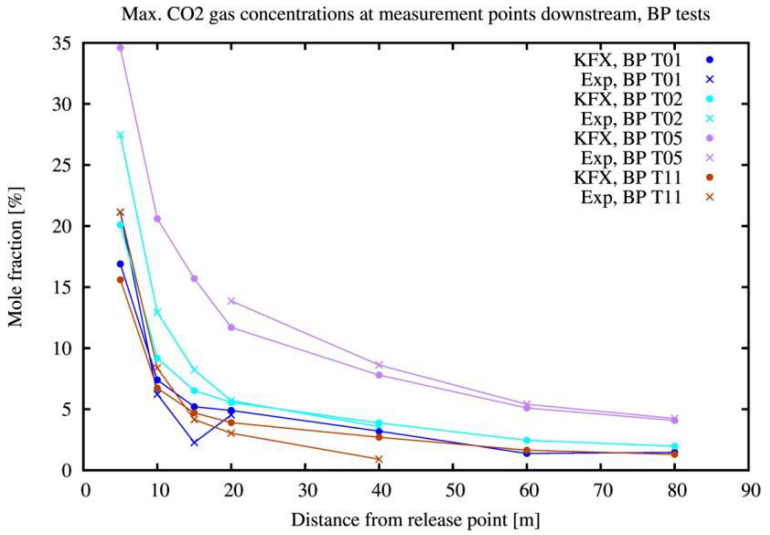

Fig. 6. Predicted and measured maximum mole fractions of CO_2 (%) versus downstream distance for the BP tests.

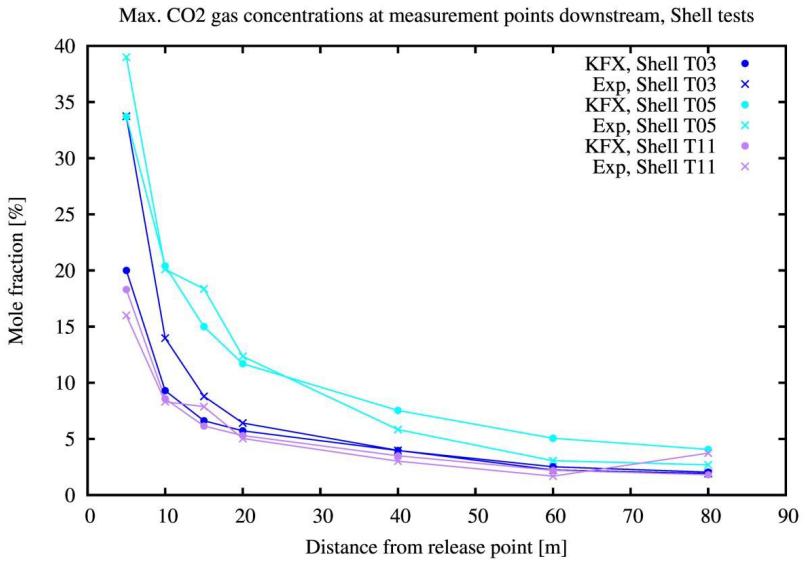

Fig. 7. Predicted and measured maximum mole fractions of CO_2 (%) versus downstream distance for the Shell tests.

The overall agreement between the predicted and measured maximum mole fractions of CO_2 is considered to be very good, cf. Fig. 6 and Fig. 7.

The deviations observed between the predicted and measured maximum mole fractions of CO_2 in the near field, close to the release point, are probably due to the simplified modeling of the flow expansion zone by the pseudo-source model. The pseudo-source model does not resolve the details of the complex multiphase flow structure of the near-field expansion process. By applying a pseudo-source concept, equivalent release conditions at atmospheric pressure are calculated at subgrid level using comprehensive CO_2 thermodynamics and fundamental conservation laws for mass, momentum and energy. This method can typically be beneficial for practical engineering dispersion simulations of high-pressure releases, but at the cost of prediction inaccuracies in the near field. On the other hand, there are also very large spatial concentration gradients in the near-field region, and small differences in the spatial location of the release orifice and logging points in the experiments and the simulations may give significant differences in concentrations.

Differences between the wind conditions in the experiments and the wind input conditions in the simulation together with the modeling of the ground can have a significant effect on the CO_2 concentrations found farther downstream. For each test, a measured averaged wind speed and direction was used as input for the specification of the logarithmic wind profile in the simulation.

Another possible reason for differences in predicted and measured CO_2 concentrations farther downstream may be strong anisotropic turbulence effects for the gas cloud flow along the ground which are not captured by the standard k-epsilon turbulence model.

Large-scale field experiments are far from trivial, and it is not always easy to say if differences in results between measurements and predictions are due to modeling errors or experimental errors and/or lack of data. For example, it could be noted that the mass balance was always met in the simulations, but impossible to control in the experimental data. In a review of the Shell CO_2 experiments where the performance of the O_2 sensors was compared against Servomex and Draeger CO_2 sensors, Witlox [14] stated that there appears to be an inherent inaccuracy for the measurements, and "as a result too high accuracy of the models (say less than 25% or 50% deviation) cannot be demanded". From a general modeling perspective, a major challenge when comparing CFD simulations to large-scale dispersion experiments is to have access to and control of all relevant input data from the experiments needed for the modeling.

4.4. Simulation of an accidental CO_2 release and subsequent dispersion in realistic terrain

Here an example of a KFX™ simulation of an accidental release of CO_2 into realistic terrain is given. For this scenario, an electronic map of the terrain was imported into KFX™ and automatically converted to a KFX™ geometry model. Liquid CO_2 at 80 bar and 280 K was released horizontally into the surroundings under low-wind conditions (0.5 m/s in the release direction, 10 m above the ground), and the nominal mass flow rate was 103 kg/s. This resulted in a cold, dense jet flow of CO_2 following the ground. In Fig. 8 and Fig. 9, the predicted iso-surface of 1 mol % CO_2 gas is shown at 28 s and at 200 s after the release started, respectively.

The elevated front of the CO_2 cloud is clearly seen in Fig. 8, and effects of the terrain on the CO_2 dispersion are demonstrated in both Fig. 8 and Fig. 9.

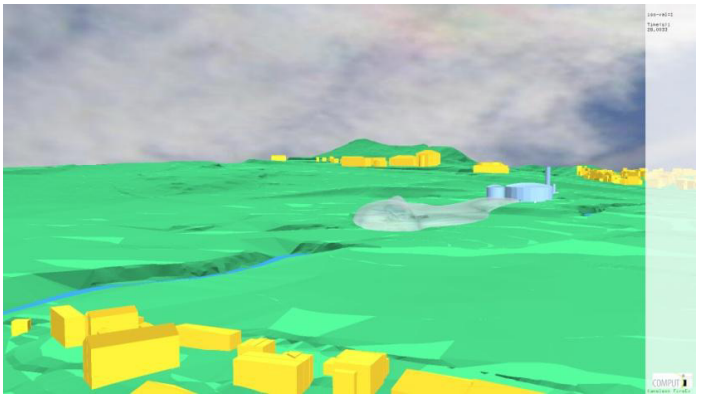

Fig. 8. Predicted 1 mol % iso-surface of CO_2 gas, 28 s after the release started.

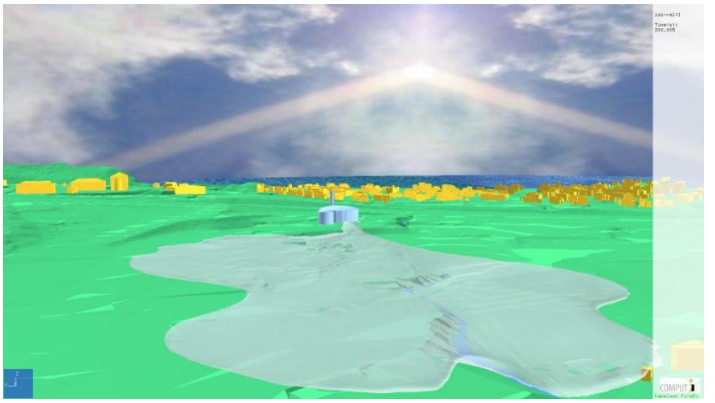

Fig. 9. Predicted 1 mol % iso-surface of CO_2 gas, 200 s after the release started.

5. Conclusion

By utilization of advanced simulation technology in design, construction and operation of CCS plants and infrastructure, CCS safety can be significantly improved and potential hazards and negative environmental impacts from the CCS industry can be reduced or eliminated in a cost-effective way. Here the development of an advanced industrial CO_2 dispersion tool for realistic conditions has been discussed and demonstrated. Validation results show that KAMELEON FIREEX KFX® is capable of producing reliable predictions of CO_2 dispersion from vents and accidental releases.

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